Butanedioic acid, 2,2,3,3-tetrafluoro-
377-38-8 | DTXSID8059928

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.11

Global applicability domain: Inside

Local applicability domain index: 4.83e-01

Confidence level: 7.54e-01

Nearest Neighbors from the Training Set

Image not found
Ethyl trifluoroacetate
Measured: 1.18
Predicted: 1.04

Image not found
Benzene, (trimethoxymethyl)-
Measured: 2.27
Predicted: 2.03

Image not found
Acetic acid, difluoro-, ethyl ester
Measured: 0.87
Predicted: 8.28e-01

Image not found
1-Methoxy-2-propyl acetate
Measured: 0.56
Predicted: 4.87e-01

Image not found
Acetic acid, trifluoro-, methyl ester
Measured: 0.6
Predicted: 7.19e-01